ON THE EQUATION OF MOTION OF THERMODYNAMICS

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ABSTRACT

Hatsopoulos and Gyftopoulos (1976a-d) argued persuasively that both Newton's equation F = ma, and von Neumann's equation $\partial \rho / \partial t = (2\pi/ih) \left[H.\rho \right]$ are incomplete, and that some nonunitary principle of quantal motion must be devised to achieve a unification of thermodynamics and quantum physics into a self-consistent theory. The two equations of motion are incomplete because they describe neither all reversible adiabatic changes of state nor any irreversible adiabatic changes of state.

Motivated either by these thermodynamic considerations or by other objectives, various authors have considered many mathematical generalizations of quantum dynamics. Are all these generalizations acceptable?

To answer this question (Çubukçu, 1993), we establish nine sensible criteria that must be satisfied by any relation purporting to represent the complete equation of motion of thermodynamics, apply these criteria to each of the proposed generalizations of von Neumann's equation, and find that the only acceptable relation is the one proposed by Beretta et al. (1984, 1985).

Nomenclature

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Α	linear operator on H or system A
a	acceleration
В	linear operator on H or system B
AB	composite of A + B
A_{xy}	kernel of operator $A = \langle \delta_x A \delta_y \rangle$
F	force
$F(\epsilon, \rho)$	linear operator on H, function of ε and ρ
$G_{\mathbf{j}}$	generators of motion (set of linear operators on H)
h	Planck's constant
H	Hamiltonian operator
H	Separable Hilbert space
i	$\sqrt{-1}$

Boltzman's constant

L	linear super-operator on L ¹ (H)
m	mass
Ni	number operator of constituent i
p	momentum operator on H
S	entropy operator on H
ŧ	time
Tr	trace of operator that follows
V_n	linear operator on H
X	position operator on H
X*	adjoint of operator X
<x></x>	expactation value of operator X
[X,Y]	
	anti-commutator of operators X and $Y = XY+YX$
δ_i	Dirac delta function
ε	set of instantaneous expressions corresponding to
	properties
γ	positive time constant
λ	positive time constant
π	the number $pi = 3.14159$
ρ	density operator
ρ ρ	density operator of a stable equilibrium state
Σ	the operator on $H = -Log(\rho)$
τ	positive time constant
τ_{i}	positive time constant of constituent i
ψ	wave function
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Dynamics

The power of a physical theory is in its ability to make predictions. A successful theory must be able to describe all types of time evolutions of systems we observe in nature, including irreversible and all forms of reversible adiabatic changes of state. In that respect, both classical and quantum mechanics are physical theories which describe only a special class of adiabatic changes of state and, hence, both Newton's equation F = ma and

Schrödinger's equation $\frac{\partial \psi}{\partial t} = \frac{2\pi}{ih}H\psi$ are incomplete. Also, it is well known that von Neumann's equation

$$\frac{\partial \rho}{\partial t} = \left(\frac{2\pi}{ih}\right) [H, \rho] = \left(\frac{2\pi}{ih}\right) (H\rho - \rho H) \tag{1}$$

implies a unitary time evolution, hence cannot describe all adiabatic changes of state (Wehrl, 1978). Hatsopoulos and Gyftopoulos (1976a-d) argued persuasively that to achieve a unification of thermodynamics and quantum physics into a self-consistent theory, some nonunitary principle of quantal motion must be devised. This new principle of equation of motion, which we call the complete equation of motion of thermodynamics, will not only describe irreversible adiabatic changes of state, but also reversible adiabatic changes of state which are not unitary.

To date, several authors have proposed many mathematical generalizations of quantal dynamics. Even though the motivation behind each such generalization is not always identical to that of Hatsopoulos and Gyftopoulos, the proposed equations of motion are candidates for being the complete equation of motion of quantum thermodynamics. In this study, we investigate whether all these generalizations are acceptable, i.e., are consistent with experimental observations and do not lead to mathematical inconsistencies.

Using thermodynamic considerations only, we establish nine sensible criteria which must be satisfied by the complete equation of motion of thermodynamics. Applying these criteria to each of the proposed mathematical generalizations of quantum dynamics, we conclude that only the equation proposed by Beretta et al. (1984, 1985) is acceptable.

Conditions Imposed on the Equation of Motion

In quantum thermodynamics the state is represented by the set ϵ of instantaneous expressions corresponding to properties and the density operator ρ . The operator ρ is a self-adjoint, non-negative definite, unit trace, linear operator on a Hilbert space H. Therefore, in dynamics, we have to describe the time evolution of both the set ϵ and the density operator ρ . In isolated systems, the set ϵ is time invariant, and so all we need is an equation that describes the time evolution of ρ . We call it the equation of motion of quantum thermodynamics.

If system A interacts with other systems, we need to describe the evolution of the set ε_A as well. One possible approach is to study the behavior of the isolated composite system A+B, where B is the union of all systems interacting with the system A. Then, the set ε_{AB} is time independent, and the time evolution of the density operator ρ_{AB} of the composite system is determined by the equation of motion for the composite system. In principle, the set ε_A and the density operator ρ_A at any instant of time t, can be recovered from the state

 $\{\varepsilon_{AB}, \rho_{AB}\}\$ of the composite at time t, provided that A is an identifiable subsystem of A+B.

The dynamical law of quantum thermodynamics remains to be established. Nevertheless, we can determine several mathematical conditions that need to be satisfied by the equation of motion.

As a first condition, we believe that the equation of motion should be compatible with the principle of determinism, i.e., without any ambiguity it should allow us to determine the state at any instant of time, given the state at some specific time. The simplest form of equation possessing this feature has the mathematical representation:

$$\frac{\partial \rho}{\partial t} = F(\varepsilon, \rho), \tag{2}$$

where $F(\varepsilon,\rho)$ is a linear operator which is a function of the state $\{\varepsilon,\rho\}$ and remains to be discovered. Note that the equations of motion of both classical and quantum mechanics have the form of Equation (2).

To be an acceptable equation of motion in the framework of quantum thermodynamics, the following mathematical conditions must be satisfied.

- 1. The equation must preserve the Hermiticity of ρ . Accordingly, $F(\varepsilon,\rho)=F^*(\varepsilon,\rho)$, where $F^*(\varepsilon,\rho)$ denotes the adjoint of the operator $F(\varepsilon,\rho)$.
- 2. The equation must preserve the trace of ρ , i.e., $Tr(\rho)=1$ at any instant of time t. Accordingly, $\frac{d}{dt}Tr(\rho)=0=Tr(F(\epsilon,\rho))$.
- 3. In an isolated system, energy must be conserved, i.e., $\frac{d}{dt}(H) = 0$, where H is the Hamiltonian operator of the system. Accordingly, $Tr(HF(\varepsilon,\rho))=0$.
- 4. The entropy of an isolated is given by $\langle S \rangle = -k \operatorname{Tr}(\rho \operatorname{Log}(\rho))$. This value must not decrease, i.e., $\frac{d}{dt}\langle S \rangle = -k \operatorname{Tr}(\operatorname{Log}(\rho)\operatorname{F}(\epsilon,\rho)) \ge 0$. Furthermore, there must exist a class of states for which the inequality becomes strict, i.e., the entropy increases, so that the equation can describe irreversible spontaneous processes which are part of innumerable experiences.
- 5. The equation should preserve the non-negative definiteness of ρ .
- 6. The equation should reduce to the von Neumann equation (Equation (1)) or, equivalently, to the Schrödinger equation $\frac{\partial \psi}{\partial t} = \frac{2\pi}{ih} H \psi \text{ if } \rho \text{ is a projector } (\rho^2 = \rho), \text{ because ordinary quantum mechanics is a special case of quantum thermodynamics.}$
- 7. Solutions of the equation for a composite of two independent systems A and B should be compatible with the two equations of motion for the parts A and B. If $\rho_{AB}(t)$ denotes the solution of the equation for the

composite system for the initial condition $\rho_{AB}(0)=\rho_A(0)\otimes\rho_B(0)$, $\rho_A(t)$ and $\rho_B(t)$ denote the solutions for the initial conditions $\rho_A(0)$ and $\rho_B(0)$, respectively, then we must have $\rho_{AB}(t)=\rho_A(t)\otimes\rho_B(t)$. This condition implies that the operator $F(\varepsilon,\rho)$ of Equation (2) must satisfy the relation: $F_{AB}(\varepsilon_{AB},\rho_{AB})=F_A(\varepsilon_A,\rho_A)\otimes\rho_B+\rho_A\otimes F_B(\varepsilon_B,\rho_B)$.

- 8. The solution of Equation (2) must exist and be unique for any initial condition $\rho(0)$.
- 9. The time evolution predicted by the equation must be consistent with experimental observations. Actually, this is the only way the equation of motion of any physical theory can be and is validated.

Candidate Equations

Many attempts have been made to establish equations that describe quantum dissipative phenomena within the framework of statistical quantum mechanics. One group consists in introducing nonlinear terms in the Schrödinger equation (Kostin, 1972, 1975; Scuch et al., 1983a-c; Gisin, 1983a-b, 1986; Albrecht, 1975; Hasse, 1975). Each proposal in this group, however, fails to satisfy Criterion 4 because it preserves the value of entropy for all adiabatic changes of state, and, therefore, is not acceptable. Accordingly, in this study we present only equations of motion which apply not only if $\rho = \rho^2$ but also if $\rho \neq \rho^2$.

The first equation of motion for the density operator ρ was proposed by von Neumann (Equation (1)). In this equation, however, ρ is interpreted as a statistical average over many projectors. Only Jauch (1968) considered all density operators $\rho=\rho^2$ and $\rho\neq\rho^2$, and postulated that the dynamical law of generalized quantum mechanics is given by the von Neumann equation. Later, Hatsopoulos and Gyftopoulos (1976a-d) postulated that the von Neumann equation applies to all density operators, $\rho=\rho^2$ and $\rho\neq\rho^2$, but only for unitary changes of ρ , and provided that ρ is represented physically (as opposed to mathematically) by a homogeneous ensemble. A homogeneous ensemble is defined as an ensemble of identical systems each of which is in a state $\{\epsilon,\rho\}$. This is a generalization of the concept of homogeneous ensemble introduced by von Neumann for the representation of a projector (wave function).

In the literature there are attempts to describe quantum dissipative phenomena using subsystem dynamics. For example, several equations of motion for the statistical operator of a subsystem have been developed by Kossakowski (1973), Lindblad (1976), and Gorini et al. (1976). These equations are based on the notion of a quantum dynamical semi-group, are derived by using the concept of "complete positivity" (Gorini, 1976; Messer and Baumgartner, 1978), and are linear in ρ. Each is of the form

$$\frac{\partial \rho}{\partial t} = L\rho, \tag{3}$$

where L is a linear operator on L¹(H), that is the Banach space over the field of real numbers of self-adjoint trace class linear operators on the Hilbert space H. The operator L is sometimes referred to as a super-operator. Because of its similarity with the Liouville equation of classical mechanics, Equation (3) is commonly referred to as the "Liouville equation".

Kossakowski's proposal is exclusively for a two-level system, and that of Gorini et al. applies to systems associated only with a finite dimensional Hilbert space H. The equation proposed by Lindblad is valid for all systems, and reduces to the equations proposed by Kossakowski and Gorini et al. Therefore, in this study, we investigate only the equation of motion proposed by Lindblad (1976) who considered a super-operator L such that

$$\frac{\partial \rho}{\partial t} = \frac{2\pi}{i\hbar} [H, \rho] + \sum_{n} \left(V_{n} \rho V_{n}^{*} - \frac{1}{2} \left\{ V_{n}^{*} V_{n}, \rho \right\}_{+} \right)$$
(4)

where
$$\left\{V_n^*V_n,\rho\right\}_+ = V_n^*V_n\rho + \rho V_n^*V_n$$
, and $\left\{V_n\right\}$ is a set

of bounded linear operators on \mathbb{H} . In the following section, we investigate whether this equation is suitable for quantum thermodynamics, even if we interprete ρ as a density operator rather than a statistical operator.

Messer and Baumgartner (1978) proposed two different equations of motion for the density operator, both nonlinear in ρ . The most important aspect of their work is the recognition that ρ cannot represent a statistical operator. They proposed these equations as a generalization of nonlinear Schrödinger equations which are valid only for projectors or wavefunctions, i.e., $\rho = \rho^2$.

The first equation proposed by Messer and Baumgartner is of the form

$$\frac{\partial \rho}{\partial t} = \frac{2\pi}{i\hbar} [H, \rho] - \frac{1}{2} \gamma (V(\rho) \sqrt{\rho} + \sqrt{\rho} V(\rho)), \qquad (5)$$

where γ is a positive constant, and $V(\rho)$ a linear operator such that

$$V(\rho)_{xy} = \left(\sqrt{\rho}\right)_{xy} Log \frac{\left(\sqrt{\rho}\right)_{xy}}{\left(\sqrt{\rho}\right)_{yx}},$$
 (6)

and A_{Xy} denotes the "kernel" of the operator A with respect to positions x and y. The kernel of an operator A is given by the inner product $<\delta_x|A|\delta_y>$, where δ_x and δ_y are Dirac delta functions singular at x and y, respectively.

The second equation proposed by Messer and Baumgartner is of the form

$$\left(\frac{\mathrm{ih}}{2\pi}\right)\frac{\partial\rho}{\partial t} = [H,\rho] - \gamma\langle p\rangle[x,p],\tag{7}$$

where γ is a positive constant, and x and p are the position and momentum operators, respectively.

Park and Simmons (1981) adopted the generalized set of density operators of quantum thermodynamics, and proposed the nonlinear equation given by

$$\frac{\partial \rho}{\partial t} = \frac{2\pi}{i\hbar} [H, \rho] + \frac{1}{\lambda} (\hat{\rho}(\rho) - \rho), \tag{8}$$

where λ is a positive constant, and $\hat{\rho}(\rho)$ is the density operator of a stable equilibrium state which shares the same values of energy, amounts of constituents and parameters with ρ .

Beretta et al. (1984) proposed another nonlinear equation for ρ . To express the Beretta equation in a compact form, we define: (a) the semi-inner product

$$(A,B) = Tr(A^*B\rho) - Tr(A^*\rho)Tr(B\rho)$$
$$= \langle A^*B \rangle - \langle A^* \rangle \langle B \rangle, \qquad (9)$$

where A and B are linear, closed operators on H; and (b) the operator Σ =-Log(p) with the convention Log(0)=0 so that the entropy of the system in state $\{\varepsilon, \rho\}$ is given by

$$S(\rho) = \langle S \rangle = -k \operatorname{Tr}(\rho \operatorname{Log}(\rho)) = k \langle \Sigma \rangle. \tag{10}$$

For systems consisting of only one constituent, the Beretta equation is given by the relation

$$\frac{\partial \rho}{\partial t} = \frac{2\pi}{i\hbar} [H, \rho] + \frac{1}{2\tau} \{\rho, D(\rho)\}_{+}$$
 (11)

where

$$D(\rho) = \frac{\begin{vmatrix} \Sigma - \langle \Sigma \rangle & G_1 - \langle G_1 \rangle & \dots & G_n - \langle G_n \rangle \\ \langle G_1, \Sigma \rangle & \langle G_1, G_1 \rangle & \dots & \langle G_1, G_n \rangle \\ \dots & \dots & \dots & \dots \\ \langle G_n, \Sigma \rangle & \langle G_n, G_1 \rangle & \dots & \langle G_n, G_n \rangle \\ & & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

|...| deneotes the determinant, $\{G_j\}$ is a set of n linear, closed, self-adjoint, commuting operators on \mathbb{H} , and τ a positive time constant. The members of the set $\{G_j\}$ are called the generators of motion, and one of them is always the Hamiltonian operator.

Because it always contains the Hamiltonian, the set $\{G_j\}$ is not empty. Its cardinality depends on the system. In grand systems, i.e., systems which admit fractional expectation values of the amounts of constituents, the constituent number operators $\{N_i\}$ are also included in the

set $\{G_j\}$. Furthermore, the elements of the set $\{G_j\}$ are always linearly independent. For certain systems, the set $\{G_j\}$ contains only the Hamiltonian and Equation (12a) reduces to

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$$D(\rho) = \frac{\begin{vmatrix} \Sigma - \langle \Sigma \rangle & H - \langle H \rangle \\ (H, \Sigma) & (H, H) \end{vmatrix}}{|(H, H)|}.$$
 (12b)

For systems consisting of more than one constituent, Beretta et al. (1985) proposed a more general equation. In the general form, to ith constituent of the system, there corresponds a different time constant τ_i . However, if we assume that all time constants τ_i are identical, then the general equation reduces to Equation (11).

For certain ρ 's the denominator in Equation (12a) can vanish and Equation (11) becomes undetermined. For those ρ 's, Beretta (1985a) postulates that D(ρ) itself vanishes, and, thus, the equation reduces to the von Neumann equation.

Finally, Korsch and Steffen (1987) proposed a nonlinear equation of motion for the statistical operator ρ . Because of the nonlinearity of the equation, the authors recognize the difficulties in interpreting the meaning assigned to ρ . However, they did not state as explicitly as Messer and Baumgartner (1978) that ρ cannot be a statistical operator. The motivation behind the work of Korsch and Steffen is to describe the irreversible dissipative time evolution of a system in contact with its environment (an open system). Their equation of motion is given by

$$\frac{\partial \rho}{\partial t} = \frac{2\pi}{i\hbar} [H, \rho] + \gamma \Delta(\rho) \tag{13}$$

where γ is a constant, $\Delta(\rho)$ a nonlinear functional of ρ given by either

$$\Delta(\rho) = (\Sigma - (\Sigma))\rho \tag{14a}$$

OF

$$\Delta(\rho) = \frac{1}{2} \{A, \rho\}_{+} - \langle A \rangle \rho \tag{14b}$$

or a combination of Equations 14a and 14b, and A an operator corresponding to an additive property of the system.

The Equation of Motion

In this section, we examine which of the equations in the preceding section meet the nine conditions discussed earlier. Upon investigation, we conclude that only the Beretta equation conforms with all the conditions.

First, we observe that the von Neumann equation (Equation (1)) satisfies Conditions 1 to 3, and 5 to 8. However, because it describes only unitary transformations

in time, the von Neumann equation conserves the value of entropy and violates Condition 4. Accordingly, we conclude that the von Neumann equation is not acceptable.

The two equations of motion proposed by Messer and Baumgartner (Equations (5) and (7)) satisfy Conditions 1 and 2. However, they do not conserve the value of energy, hence violate Condition 3. Even though this last statement alone shows that the equations proposed by Messer and Baumgartner are unacceptable, for the sake of completeness, we investigate them further. The authors emphasized that the question of whether or not these equations satisfy Conditions 5 and 8 is an open one. Both equations violate Condition 6, however. They are invented in such a way that, if p is a projector, each equation reduces to a so-called "nonlinear Schrödinger equation" instead of the Schrödinger equation. Furthermore, it is not known whether or not Equation (5) satisfies Condition 4. It is easy to show that Equation (7) conserves the value of entropy, and therefore violates Condition 4. Based on these observations, we conclude that both equations proposed by Messer and Baumgartner are not acceptable.

Simmons and Park (1981a-b) have criticized the way the Liouville equations are derived for the statistical operator. Here, we are not interested in how the equations are derived, but rather in whether they satisfy Conditions 1 to 9. It turns out that the Liouville equations do not satisfy these conditions.

If it were possible to find a Liouville equation that satisfies the Conditions 1 to 9, we could have postulated it as being the equation of motion of quantum thermodynamics by interpreting p as a density operator. This approach would have been fundamentally different from those of Lindblad, Kossakowski and Gorini who "derived" rather than "postulated" their equation. It is noteworthy, however, that if the equation of motion cannot be derived from known principles because these principles do not regularize all experiences, then it must be postulated.

It is easy to verify that the Lindblad equation satisfies Conditions 1 and 2. The first difficulty encountered with the Liouville equations proposed in the literature is that, in general, they are not energy conserving and do not conform with the principle of entropy non-decrease (Park and Simmons, 1981; Simmons and Park, 1981). It is possible, however, to give a version of the Lindblad equation (Equation (4)) which is both energy conserving and entropy non-decreasing, for the special case of a twolevel system. Therefore, we cannot find a definitive answer to the question of whether or not, with a proper choice of $\{V_n\}$, the Lindblad equation satisfies Conditions 3 and 4. It can be readily shown, however, that the Lindblad equation does not satisfy Condition 5, because it preserves the non-negativity of the density operator only in the positive direction in time. Given the state of a system at an instant of time t, in a deterministic theory, the state at any other instant of time (both after and before t) is uniquely determined. The Lindblad equation fails to

satisfy this criterion because it does not preserve the nonnegativity of the density operator in the negative direction in time and, therefore, we cannot recover the state of the system in the past. Accordingly, we conclude that the Lindblad equation is not suitable for our purposes.

For the sake of completeness, we also investigate whether the Lindblad equation satisfies Conditions 6 to 9. Condition 8 is satisfied because Lindblad (1976) used it in deriving his equation. Qubukçu (1993) has shown that the Lindblad equation does not comply with Conditions 6 and 9, and Condition 7 is satisfied only with a proper choice of $\{V_n\}$. From this discussion, we conclude that the Lindblad equation is not acceptable.

Park and Band (1977, 1978a-b) searched for a generalized equation of motion linear in p which takes any initial state to a stable equilibrium state with the same values of energy, amounts of constituents and parameters as the initial state. They have found that such an equation exists for two-level systems. However, later on Simmons and Park (1981a) showed that no such linear equation exists for N-level systems with N>2, and concluded that any equation of motion which takes a state to its corresponding stable equilibrium state must be nonlinear in o. They have proposed Equation (8), which clearly satisfies their criterion, and have shown that it satisfies Conditions 1 to 4. Because $\hat{\rho}(\rho)$ is determined once the initial density operator is given, Condition 8 is also satisfied. The reason is that then the equation becomes linear in o and its solutions are known to exist and be unique (Bender and Orszag, 1978). However, the Park-Simmons equation satisfies Condition 7 only in an artificial manner. It is clear that the equation for a composite system takes any initial state to a stable equilibrium state of the composite system in which the individual parts are in mutual stable equilibrium with each other. However, if the equation is solved for each individual part, the resulting stable equilibrium states of the parts are not necessarily in mutual stable equilibrium. For example, the temperatures of the final states are not necessarily identical. There is no reason for them to be identical because the parts are independent of each other. The difficulty can be avoided only by postulating that a system should first be decomposed to its independent parts and then the Park-Simmons equation be applied to each part. Even if the problem with Condition 7 is resolved, Cubukçu (1993) has shown that the equation violates Conditions 5, 6 and 9 exactly in the same manner as the Lindblad equation. Accordingly, we conclude that the Park-Simmons equation is not acceptable.

The Beretta equation (Equation (11)) is the most promising among the candidate generalizations of quantum dynamics. Beretta et al. (1984) showed that his equation satisfies Conditions 1 to 6. Cubukçu (1993) has shown that the equation satisfies Condition 7 as well. The major difficulty to date has been to prove the existence and uniqueness of the solutions of the equation, but as shown by Cubukçu (1993), this difficulty has been resolved and

the Beretta equation satisfies Condition 8. In principle, the equation describes both reversible and irreversible spontaneous processes (Beretta et al., 1984), i.e., processes in isolated systems. Because it reduces to the Schrödinger equation or, equivalently, to the von Neumann equation for mechanical states, the Beretta equation describes all the processes captured by either of these two equations. The validity of the equation for the more general states ($p \neq p^2$) remains to be shown. We suggest a number of experiments which can validate quantitatively this equation and which can be used to evaluate the time constant τ (Çubukçu, 1993). Beretta (1985a-b) also suggested an experiment for a quantitative verification of his equation of motion.

Korsch and Steffen (1987) introduced their equation in the context of subsystem dynamics. In its general form the equation results in entropy increase if initially the state is not equilibrium. Upon requiring that energy be conserved, Korsch and Steffen showed that their equation reduces to the Beretta equation, and concluded that the latter is the most general equation that satisfies all the requirements of quantum thermodynamics.

Because the Beretta equation is the only equation which complies with all the conditions we have determined, we concur with the conclusions of Korsch and Steffen.

Conclusion

Hatsopoulos and Gyftopoulos (1976a-d) have developed a new physical theory which encompasses both thermodynamics and mechanics within a single mathematical framework, called quantum thermodynamics, without use of statistical mechanics. This theory describes all reversible and irreversible adiabatic changes of state. The complete equation of motion of quantum thermodynamics remains to be discovered, however. To determine the complete equation of motion, in this paper we investigate whether the generalizations of quantum dynamics proposed in the literature satisfy the set of requirements we have established from thermodynamic considerations only. Upon this investigation, we conclude that only the equation of motion proposed by Beretta et al. (1984, 1985) satisfies all the established criteria.

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